

I U C L I D

Data Set

Existing Chemical : ID: 16883-83-3
Memo : HPV Chemical
CAS No. : 16883-83-3
TSCA Name : 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Molecular Formula : C27H34O6
Product name : Texanol benzyl phthalate

Producer related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 18.10.2000

Substance related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 18.10.2000

Status :
Memo : ACC Phthalate Ester Panel HPV Testing Group

Printing date : 07.12.2006
Revision date :
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Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 16883-83-3
Date 07.12.2006

1.0.1 APPLICANT AND COMPANY INFORMATION

Type : lead organisation
Name : ACC Phthalate Esters Panel HPV Testing Group
Contact person : Dr. Marian Stanley
Date :
Street : 1300 Wilson Blvd.
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Homepage :

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes eleven CAS numbers (see the Freetext Remark section for complete list).

Remark : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. The subcategory includes the following eleven CAS numbers:
68648-93-1 1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)

117-84-0 1,2,-benzenedicarboxylic acid, dioctyl ester (DOP)

16883-83-3 1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)

68515-40-2 1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)

68515-45-7 1,2,-benzenedicarboxylic acid, dinonyl ester, branched and

linear (DNP)

68515-43-5 1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)

84-77-5 1,2-benzenedicarboxylic acid, didecyl ester (DDP)

3648-20-2 1,2-benzenedicarboxylic acid, diundecyl ester (DUP)

85507-79-5 1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)

111381-91-0 1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)

68515-47-9 1,2,-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250°C) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including di-isononyl (DINP) and di-isodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

08.05.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :

1. General Information

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Substance type : organic
Physical status : liquid
Purity :
Colour :
Odour :

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Polymers industry

Remark : High molecular weight phthalates are used nearly exclusively as plasticizers of PVC.

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 16883-83-3

Date 07.12.2006

2.1 MELTING POINT

Value	: -6.5 °C
Decomposition	: no, at °C
Sublimation	:
Method	: other: no data
Year	:
GLP	:
Test substance	: other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Remark	: Data are from manufacturer's product profile.
Test substance	: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Reliability	: (2) valid with restrictions This robust summary is assigned a reliability of 2 because there is limited information on how the data were developed.
Flag	: Critical study for SIDS endpoint
31.05.2006	(5)
Value	: 152 °C
Decomposition	: no, at °C
Sublimation	: no
Method	: other: calculation
Year	:
GLP	:
Test substance	: other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Method	: Melting point calculation by MPBPWIN ver. 1.41 using calculation methods of Joback and Gold and Ogle.
Remark	: EPI Suite™ is used and advocated by the US EPA for chemical property estimation. However, the melting point calculation in EPI Suite™ gives erroneously high results for the phthalate esters.
Test substance	: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Reliability	: (3) invalid
31.05.2006	(5)

2.2 BOILING POINT

Value	: 474 °C at 1013 hPa
Decomposition	: no
Method	: other
Year	:
GLP	:
Test substance	: other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Method	: Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown.
Remark	: EPI Suite™ is used and advocated by the US EPA for chemical property estimation.
Test substance	: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Reliability	: (2) valid with restrictions This robust summary has a reliability rating of 2 because the data are

2. Physico-Chemical Data

Id 16883-83-3

Date 07.12.2006

Flag : calculated.
31.05.2006 : Critical study for SIDS endpoint (5)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .00000000848 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Method : Vapor pressure calculation by MPBPWIN ver. 1.41 using calculation method of Grain.
Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
31.05.2006 (5)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : 7 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Method : Partition coefficient by LOGKOWWIN ver. 1.67 using an atom/fragment calculation method of Meylan and Howard.
Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
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2. Physico-Chemical Data

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2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : .00147 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Method : Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 8.54.

Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.

Test substance : CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
31.05.2006 (5)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

Id 16883-83-3

Date 07.12.2006

3.1.1 PHOTODEGRADATION

Type : air
Light source : Sun light
Light spectrum : nm
Relative intensity : 1 based on intensity of sunlight
Conc. of substance : at 25 °C
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : .0000000001727 cm³/(molecule*sec)
Degradation : 50 % after 7.4 hour(s)
Deg. product : not measured
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Method : Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.
Remark : 50% degradation after 7.43 hrs or 0.62 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration.
EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
07.12.2006

(5)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : 1.6 year at 25 °C
t1/2 pH9 : at °C
Deg. product : not measured
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Method : Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark : EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

3. Environmental Fate and Pathways

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Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
06.07.2006

(5)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
-----------	----------------

Molecular Weight	454.57
Temperature	25° C
Log Kow	7.0
Water Solubility	0.00147 g/m3
Vapor Pressure	0.000000848 Pa
Melting Point	-6.5°C

Result : Using the Mackay Level I calculation, the following distribution is predicted for benzyl octylbutyl phthalate:

% Distribution	Compartment
0.0	Air
0.0	Water
97.7	Soil
2.2	Sediment
0.1	Suspended Sediment
0.0	Biota

Test substance : CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
02.06.2006

(6)

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Remark : Physicochemical data used in the calculation:

3. Environmental Fate and Pathways

Id 16883-83-3

Date 07.12.2006

Parameter	Value w/ Units
-----------	----------------

Molecular Weight	454.57
Temperature	25° C
Log Kow	7.0
Water Solubility	0.00147 g/m3
Vapor Pressure	0.000000848 Pa
Melting Point	-6.5°C

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
-------------	--------------

Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
-------------	----------------

Air	14.8a
Water	120b
Soil	420c
Sediment	420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI Suite™ version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI Suite™, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from: Sugatt et al (1983, 1984), CITI (1992), and Boethling (2000).
Sugatt R et al., (1983). Shake Flask Biodegradation of 14 Commercial Phthalate Esters. Syracuse Research Corporation, Syracuse, NY. SRC# L1543-05.

Sugatt R, O'Grady D, Banerjee S, Howard P and Gledhill W (1984). Shake flask biodegradation of 14 commercial phthalate esters. App. Environ. Microbiol. 47, 601-606.

CITI (Chemicals Inspection & Testing Institute) (1992). Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL Japan. Japan Chemical Industry Ecology-Toxicology & Information Center.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Result

: Using the Mackay Level III calculation, the following distribution is predicted for benzyl octylbutyl phthalate:

Compartment	% Distribution
Air	1.0
Water	8.5
Soil	70.2

3. Environmental Fate and Pathways

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Test substance : Sediment 20.3
: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
No information on purity.

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
02.06.2006 (6)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4. Ecotoxicity

Id 16883-83-3

Date 07.12.2006

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Pimephales promelas (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : > 1000
Limit test : yes
Analytical monitoring : no
Method : other: EPA-600/3-75-009
Year : 1975
GLP : yes
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Method : Method/Guideline - USEPA, (EPA-600/3-75-009), Methods for Acute Toxicity tests with Fish, Macroinvertebrates and Amphibians; 1975
Statistical methods - NA

Result : No mortality was observed at highest loading level, 1000 mg/L.

An oily sheen was observed on the surface of the 1000 mg/L test treatments after test substance addition. Test treatment level was above water solubility value.

At 24 hours, test solution (control and 1000 mg/L) dissolved oxygen was low and the solutions were aerated for the study duration at sponsor's request.

Test condition : Fish mean total length = 38.4 mm, mean wet weight = 0.89 g, organism loading was not calculated.
A limit test consisting of one test treatment and control was performed. The test treatment was prepared at a loading of 1000 mg/L. The test substance was added directly to 5 gallon glass replicate vessels containing 15 liters of dilution water. One replicate of the control and two replicates of the test treatment were evaluated. Each test vessel contained 10 fish. Dilution water was filtered well water.

Test temperature = 22 +/- 1 Deg C.,
The pH range was 7.7 to 8.3. The Dissolved oxygen ranged from 4.2 to 8.7 mg/L. Fish were obtained from Fender's Fish Hatchery in Baltic, Ohio.

Test substance : Nominal test concentrations: Control, and 1000 mg/L.
1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3)
No information on purity.

Conclusion : Test substance is non-toxic to fish at or below its water solubility level.
Reliability : (2) valid with restrictions

This study is rated a "2" because there is limited information on treatment solution preparation and water quality parameters.

Flag : Critical study for SIDS endpoint
06.07.2006

(1)

Type : static
Species : Salmo gairdneri (Fish, estuary, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LC50 : > 1000
Limit test : yes
Analytical monitoring : no
Method : other: EPA-600/3-75-009

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Year : 1975
GLP : no
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Method : Method/Guideline - USEPA, (EPA-600/3-75-009), Methods for Acute Toxicity tests with Fish, Macroinvertebrates and Amphibians; 1975
Statistical methods - NA
Result : No mortality was observed at highest loading level, 1000 mg/L.
Test treatment level was above water solubility value.
Test condition : 10 fish per vessels were employed in 5 gallon glass aquaria containing 15 liters of water. Water parameters were; DO = 8.9 mg/L; pH = 7.8. total hardness = 240 mg/L CaCO₃, total alkalinity = 360 mg/L CaCO₃ Testing temperature was 22°C. Fish were acclimated and held without food for 48 hours prior to testing. Exposure was to a single dose level of 1000 mg test material /L. A positive control, antimycin A, was used.
Test concentrations: Control, and 1000 mg/L.
Test substance : 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3)
No information on purity.
Conclusion : Test substance is non-toxic to fish at or below its water solubility level.
Reliability : (2) valid with restrictions
This study is rated a "2" because there is limited information on treatment solution preparation and water quality parameters.
Flag : Critical study for SIDS endpoint
15.11.2006 (1)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
LC50 : 7.5
Analytical monitoring : no
Method : other: EPA-660/3-75-009
Year : 1975
GLP : yes
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Method : Method/Guideline - USEPA, (EPA-660/3-75-009) Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians; 1975
Statistical methods - Moving average angle, Probit or Binomial
Result : There were limited details describing the treatment preparation phase.

Nominal test concentrations:

Loading Level (mg/L)	Mortality (48 h)
Control	0
Solvent Control	0
1.0	0
1.8	0
3.2	0
5.6	3
10.0	17

Test condition : Value - 7.5 mg/L (CI of 6.6 to 8.5) based upon nominal loading levels.
Test treatments were prepared by adding the test substance with acetone directly to the test treatments. The acetone control and high concentration (10 mg/L) each contained 1.0 ml of acetone for each 200 ml replicate. All

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other treatment replicates contained a lesser, yet proportional amount of acetone. Two replicates of ten organisms were tested per treatment. Test vessels were 250 ml beakers with 200 ml of test solution. The dilution water was well water with a hardness of 255 mg/L as CaCO₃ and an alkalinity of 368 mg/L as CaCO₃.

Test temperature=20 +/- 1 Deg C.,

The pH ranged from 7.8 to 7.9 during the study. Dissolved Oxygen was 9.2 mg/L. Daphnia were <24 hours old and obtained from in-house stock. Lighting was 16 hours light and 8 hours dark (no intensity reported).

Nominal test concentrations: Loading Level (mg/L) Control, Solvent Control, 1.0, 1.8, 3.2, 5.6, 10.0

Test substance : 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3)
No information on purity.

Reliability : (3) invalid
This study is rated a "3" because the test organisms are likely to have become fouled by the test material.

06.07.2006

(2)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : *Selenastrum capricornutum* (Algae)

Endpoint :

Exposure period : 96 hour(s)

Unit : mg/l

EC50 : > 1000

Limit test :

Analytical monitoring : no

Method : other

Year : 1971

GLP : yes

Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Method : Method/Guideline - U.S. EPA, Algal Assay Procedure: Bottle Test, 1971.
Test type-Static Acute
Statistical methods-NA

Result : In-vivo chlorophyll a, measured daily. Both cell numbers and in-vivo chlorophyll a, measured at termination.
Chlorophyll a measured using a Turner filter fluorometer. Cells counts performed via a hemacytometer.

% Difference at 96 hr relative to control:

Loading Level (mg/L)	Chlorophyll a	Cell #
Control	---	---
360	-22	-9
600	-22	-12
1000	-36	-21

Test condition : Value - EC50 = >1000 ppm based upon chlorophyll a and cell counts.
The appropriate amount of test substance was added directly to algal growth medium (control and diluent) to form individual treatment concentrations. The test was performed in 125 ml flasks. The initial algal concentration was not reported.

Lighting = 4,000 lux, Test temperature = 24+/-1 Deg C. The pH range was 7.2 to 7.4. Algal culture stock obtained from U.S. EPA Environmental Research Laboratory, Corvallis, Oregon.

4. Ecotoxicity

Id 16883-83-3

Date 07.12.2006

Test substance	: Nominal test concentrations: control, 360, 600, and 1000 mg/L. : 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3) : No information on purity.
Conclusion	: Test substance is not toxic to algae at or below its water solubility level.
Reliability	: (2) valid with restrictions : This study is rated a "2" because there is limited information on treatment solution preparation and water quality parameters. Also, there was no information on initial or final cell counts reported.
Flag	: Critical study for SIDS endpoint

02.06.2006 (4)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	: LD50
Value	: > 15800 mg/kg bw
Species	: rat
Strain	: Sprague-Dawley
Sex	: male/female
Number of animals	: 20
Vehicle	: no data
Doses	:
Method	: other
Year	:
GLP	: no
Test substance	: other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Method	: Single rats were used for the lower doses; 5 rats (3 male, 2 female) were used at the highest dose.
Remark	: No animals died at any dose level. Toxic signs reported as reduced appetite slight weakness for one to three days (numbers and dose levels not reported). Weight gain was normal. At necropsy, two rats at the highest dose level (15800 mg/kg) were observed with hemorrhagic areas in the lungs and all animals in the 12,600 and 15,800 mg/kg groups had gaseous intestinal tracts.
Test condition	: The undiluted test material was fed by stomach tube to rats in increasing doses at increments of fractional log intervals. The dose levels were 2000, 3160, 5010, 7940, 12600, and 15800 mg/kg. Single rats were used for the lower doses; 5 rats (3 male, 2 female) were used at the highest dose. The rats were observed for toxic signs and sacrificed after 9 days.
Test substance	: 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3)
Conclusion	: The compound was found to be non-lethal by oral ingestion in male and female rats.
Reliability	: (2) valid with restrictions
Flag	: Critical study for SIDS endpoint
07.12.2006	(7)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	: LD50
Value	: > 7940 mg/kg bw
Species	: rabbit
Strain	: New Zealand white
Sex	: male/female
Number of animals	: 5
Vehicle	: no data
Doses	:
Method	: other
Year	:
GLP	: no

Test substance	: other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Remark	: No animals died at any dose level. Toxic signs reported as reduced appetite and activity, slight lethargy (2 to 5 days) and slight tremors (1 to 2 days) in the three highest dose levels rabbits (5010, 7940 mg/kg). At necropsy, the three rabbits in the highest dose levels (5010, 7940 mg/kg) were observed with slight congestion of the lungs and areas of slight discoloration of the liver; the two rabbits at 2000 and 3160 mg/kg appeared normal.
Test condition	: The undiluted compound was applied in increasing doses at increments of 0.2 fractional log intervals to the closely clipped, intact skin of male and female rabbits. The dose levels were 2000, 3160, 5010, and 7940 mg/kg. The treated areas were covered with plastic strips and animals held in wooden stocks for up to 24 hours, after which they were held in individual cages. The rabbits were observed for toxic signs daily for seven days. Surviving animals were sacrificed after seven days and observed for macroscopic abnormalities.
Test substance	: 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3)
Conclusion	: The compound was considered practically non-toxic by dermal exposure in male and female rabbits.
Reliability	: (2) valid with restrictions
Flag	: Critical study for SIDS endpoint
07.12.2006	(8)
Type	: LD50
Value	: > 10000 - mg/kg bw
Species	: rabbit
Strain	: other: New Zealand
Sex	: male/female
Number of animals	:
Vehicle	:
Doses	:
Method	: other: not stated
Year	: 1969
GLP	: no
Test substance	: other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester
Method	: Statistical methods: None
Remark	: Test type: Skin absorption Exposure period: Single exposure followed by 14 day observation period Analytical monitoring: No
Result	: Mortality: All animals survived to necropsy Units: Mg/kg Value: Acute dermal LD50 > 10,000 mg/kg
Test condition	: One male or female rabbit per dose received a single dermal application of 2510 to 10000mg/kg test material to clipped, intact skin. The application site was covered with plastic strips for 24 hours and the animals were held for 14 days post dosing. Toxic signs and weight gain were monitored; all animals were necropsied.
Test substance	: 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3)
Conclusion	: Test material is practically acutely nontoxic dermally.
Reliability	: (2) valid with restrictions
07.12.2006	(10)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result :
Classification :
Method : other: not stated
Year : 1969
GLP : no
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Method : Dermal reaction scoring according to the method of Draize.
Statistical methods: None.

Remark : Test type: Skin irritation
Strain: New Zealand
Sex: male and female
Analytical monitoring: No
Exposure period: Single 24-hour exposure followed by 7 day observation period

Result : Erythema and edema scores not given; average maximum irritation score occurred at 24 hours post application and was 0.6 out of a possible 8.0.

Test condition : Three male or female rabbits received a single dermal application of undiluted test material to clipped, intact skin. Amount applied not stated. The application site was covered with plastic strips for 24 hours and the animals were held for 7 days post dosing.

Test substance : 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3)

Conclusion : Test material is considered nonirritating to the intact skin.

Reliability : (2) valid with restrictions

07.12.2006 (3) (10)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration :
Dose :
Exposure time :
Comment :
Number of animals :
Vehicle :
Result :
Classification :
Method : other: not stated
Year : 1969
GLP : no
Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Method : Ocular reaction scoring according to the method of Draize.
Statistical method: None

Remark : Test type: Eye irritation
Strain: New Zealand
Sex: male and female

5. Toxicity

Id 16883-83-3

Date 07.12.2006

Analytical monitoring: No
Exposure period: 0.1 ml instilled into conjunctival sac. Exposure followed by 7 day observation period.

Result : Eryhema and edema scores not given; average maximum irritation score occurred at 1 hour post application and was 4.0 out of a possible 110.0.

Test condition : Three male or female rabbits received a single instillation of undiluted test material into their conjunctival sac. 24 post application the eyes were rinsed with warm isotonic saline. Animals were held for 7 days post dosing.

Test substance : 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3)

Conclusion : 2Test material is considered slightly irritating to the eye.

Reliability : (2) valid with restrictions

07.12.2006 (3) (10)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Ames test

System of testing : Bacterial

Test concentration : 0.01, 0.04, 0.2, 1.0, 3.0, and 10.0 ul/plate

Cycotoxic concentr. :

Metabolic activation : with and without

Result : negative

Method : OECD Guide-line 471

Year :

GLP : yes

Test substance : other TS: CAS #16883-83-3; 1,2-benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester

Method : Statistical analysis was performed on the results after transforming to values to log10. Analysis included Bartlett's test for homogeneity of variance and comparison to controls with a t-test. Dose-response was evaluated with regression analysis and significance of the response evaluated by a t-test.

Remark : The substance was not mutagenic at doses < 10 mg/plate in Salmonella strains TA98, TA100, TA1535, TA1537 and TA1538 in plate incorporation assays with or without metabolic activation. No microbial toxicity was observed in any of the five strains at 10 mg/plate with or without metabolic activation, although levels of 3 ug/plate and higher exceeded the solubility of the test material.

Test condition : Positive control chemicals were sodium nitrite, 9-aminoacridine, and 4-nitroquinoline-N-oxide (without S9); or benzo(a)pyrene, 2-acetylaminofluorene, and 2-aminoanthracene (with S9); the solvent control was DMSO. Concurrent solvent and positive controls were included in all experiments. A toxicity pretest with TA 100 was conducted with and without microsomal activation to determine the highest dose level. The plate incorporation tests were conducted in all strains with and without activation.

Test substance : 1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl phenylmethyl ester (CAS# 16883-83-3)

Conclusion : The test substance was not mutagenic in all strains tested.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

06.07.2006 (9)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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- (2) Analytical Bio Chemistry Laboratories, Inc (ABC) (1979). Static Acute Bioassay No. 23221, for Monsanto Chemical Company, St. Louis, MO, USA.
- (3) Draize, J. H., J. of Pharm ad Exp. Therapeutics, Vol 38, December, 1944.
- (4) EG&G, Bionomics Marine Research Laboratory (1979). Freshwater Alga Toxicity Test with *Selenastrum capricornutum*. Report No. BP-79-4-60 for Monsanto Chemical Company, St. Louis, MO, USA.
- (5) Environmental Protection Agency (EPA) (2000). EPI Suite™, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.
- (6) Mackay D (1998). Level III Fugacity-Based Environmental Equilibrium Partitioning Model, Version 2.1 (16-bit). Environmental Modelling Centre, Trent University, Ontario, Canada.
- (7) Monsanto Company (1969). Range finding acute oral toxicity with Santicizer 278. Unpublished report.
- (8) Monsanto Company (1970). Minimum Lethal Dose by Skin Adsorption in Rabbits with Santicizer 278. Unpublished report.
- (9) Monsanto Research Corporation (1982). *Salmonella* Mutagenicity Assay of Santicizer 278. Unpublished report.
- (10) Younger Laboratories, St. Louis, MO., Toxicological Investigations of Santicizer 278, 1969.

10.1 END POINT SUMMARY**10.2 HAZARD SUMMARY**

Memo : This chemical is part of the High Molecular Weight Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the higher phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this subcategory. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physicochemical and fate properties of the HPV phthalates in the high molecular weight subcategory.

A complete health effects SIDS data set is available for diisononyl (DINP) and diisodecyl (DIDP) phthalates. These substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds for the high molecular weight phthalate subcategory. Although not complete, health effects data are also available for many of the HPV substances in this subcategory. These phthalates all demonstrate minimal acute toxicity, are not genotoxic, exhibit some liver and kidney effects at high doses, and are negative for reproductive and developmental effects. Further, the available data indicate that the toxicological activity of these molecules diminishes with increasing molecular weight. The available data, supplemented with the data from the reference compounds (DINP, DIDP), are believed to be sufficient to use as read-across to the other category members, with side chains in the C7 - C13 range.

Ecotoxicity test data in fish, daphnia, and algae are available for 610P, 711P, DINP, DUP, DIDP and DTDP. These phthalates all contain alkyl chain lengths in the range of C7 to C13. The remaining members of this subgroup are all various mixtures of C7 through C11 alkyl chain isomers. All of the measured data for these higher phthalates show no effects on acute or chronic exposure to aquatic organisms. As with DIOP and DEHP, the higher phthalates are too insoluble to have acute or chronic toxicity.

06.07.2006

10.3 RISK ASSESSMENT